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Synthesis and crystal structure of 2-(benzo[*d*]thiazol-2-yl)-*N*′-[(*E*)-1-(4-bromophenyl)ethylidene]acetohydrazide

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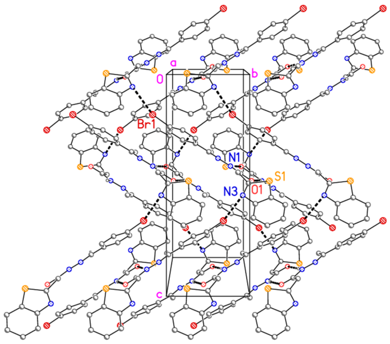
The title compound (*E*)-2-(benzo[*d*]thiazol-2-yl)-*N*′-(1-(4-bromophenyl)ethylidene)acetohydrazide, $C_{17}H_{14}BrN_3OS$, crystallizes in space group $P2_1/c$ with $Z = 4$. The configuration across the formal $N=C$ double bond at the hydrazide moiety is *E*; the atom sequence $C—C—C(=O)—N—N=C—$(bromophenyl) is very approximately planar (r.m.s. deviation 0.17 Å, when all carbon atoms of the bromophenyl group are included), being synperiplanar around the $C(=O)—N$ bond and antiperiplanar (choosing the appropriate final atom C_{Ar}) elsewhere. The interplanar angle to the benzothiazole unit (r.m.s. deviation 0.01 Å) is 69.75 (2)°. The main packing feature is a classical inversion-symmetric dimer with hydrogen bonds of the type $N—H\cdots O=C$. This combines with a rather long $N_{thiazole}\cdots Br$ halogen bond to form a thick layer structure parallel to the *bc* plane.



1. Chemical context

The benzothiazole scaffold is established as one of the most significant moieties in medicinal chemistry, because benzothiazole derivatives are present in a broad range of natural products and bioactive compounds, and many derivatives exhibit significant activity while causing few side-effects (Keri *et al.*, 2015). Benzothiazole derivatives have attracted appreciable recent attention in medicinal chemistry because of their biological and pharmacological characteristics (Gill *et al.*, 2015). Numerous biological activities, including anticancer, antifungal and antibacterial effects, are associated with the benzothiazole moiety; a more extensive description can be found in our previous publication (Elboshi *et al.*, 2026) and references therein.

We have synthesised new heterocyclic compounds with incorporated benzothiazole motifs, and these too have demonstrated noteworthy biological activity (Azzam *et al.*, 2017), *e.g.* benzothiazole-substituted coumarin residues, which also have useful optical characteristics (Abdallah *et al.*, 2023). We have described some new coumarin compounds that are currently being used as laser dyes for medicinal applications (Elgemeie, 1989). We have also reported new benzothiazole-based heterocycles that showed significant fluorescence as well as biological importance (Azzam *et al.*, 2022).

The goal of the current study was to design and produce benzothiazolyl ethylidene-acetohydrazides inspired by the results of our earlier work. The 2-(benzothiazolyl)-[1-(4-bromophenyl)ethylidene]acetohydrazide derivative **7** was synthesized in good yield by reacting 2-benzothiazolyl acetohydrazide **4** with 4-bromophenylacetophenone **5** in refluxing

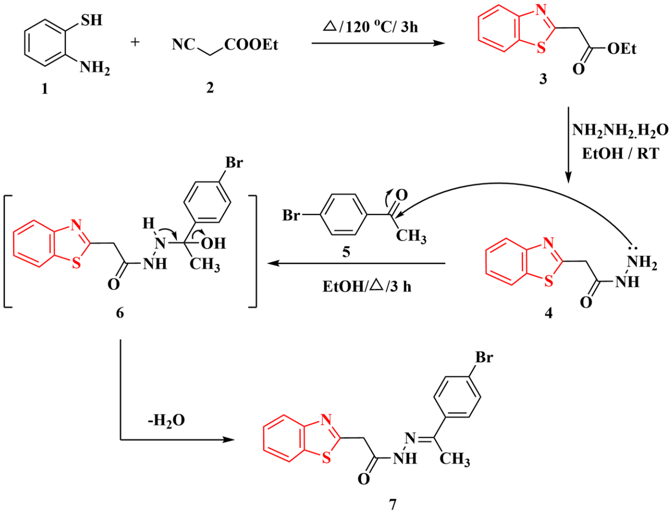


Figure 1
The synthesis of compound **7**.

ethanol for 3 h (Fig. 1). The crystal structure of **7** was determined and is reported here.

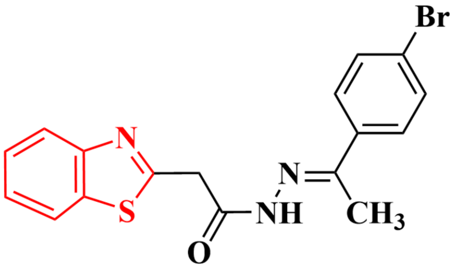


Table 1
Selected geometric parameters (Å, °).

S1—C7*A*	1.7342 (12)	C9—O1	1.2307 (15)
S1—C2	1.7507 (12)	C9—N1	1.3543 (15)
C2—N3	1.2976 (16)	N1—N2	1.3764 (15)
N3—C3*A*	1.3909 (16)	N2—C10	1.2942 (15)
C3*A*—C7*A*	1.4090 (17)		
C7*A*—S1—C2	89.24 (6)	C7—C7*A*—S1	129.27 (10)
N3—C2—S1	115.90 (9)	C3*A*—C7*A*—S1	109.07 (8)
C2—N3—C3*A*	110.63 (10)	C9—N1—N2	119.49 (10)
N3—C3*A*—C4	125.01 (11)	C10—N2—N1	116.53 (10)
N3—C3*A*—C7*A*	115.16 (10)		
N3—C2—C8—C9	−115.73 (13)	C9—N1—N2—C10	−179.12 (12)
C2—C8—C9—O1	−10.43 (19)	N1—N2—C10—C11	179.74 (11)
C2—C8—C9—N1	170.32 (12)	N2—C10—C11—C12	−160.60 (12)
C8—C9—N1—N2	−1.76 (18)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H01···O1^{i}	0.91 (2)	1.98 (2)	2.8839 (14)	168 (2)
C7—H7···N3^{ii}	0.95	2.68	3.5942 (17)	161
C17—H11*B*···Br1^{iii}	0.98	2.93	3.7666 (12)	145
C17—H11*C*···N2^{iv}	0.98	2.69	3.5464 (18)	147

Symmetry codes: (i) $-x+1, -y+2, -z+1$; (ii) $x, y+1, z$; (iii) $-x+1, y+\frac{1}{2}, -z+\frac{1}{2}$; (iv) $-x+1, -y+1, -z+1$.

2. Structural commentary

The molecule of compound **7** is shown in Fig. 2, with selected geometric parameters in Table 1. The molecular dimensions may be regarded as normal, *e.g.* the wide exocyclic angles at C3*A* and C7*A*. The configuration across the formal double bond N2═C10 is *E*, and this bond is some 0.06 Å shorter than the formal single bond N1—C9, although formal bond orders should be interpreted carefully in view of probable delocalization of the multiple bonding. The approximate synperiplanarity of the sequence C2—C8—C9—O1 is associated with the intramolecular S1···O1 contact of 3.1729 (10) Å, a feature that we have frequently observed in related compounds, generally with much shorter contact distances (*e.g.* Elboshi *et al.*, 2026). As can be seen from the side view of the molecule in Fig. 3, the atom sequence C2–C8–C9–N1–N2–C10–C11–C12 is very approximately planar (r.m.s. deviation 0.17 Å, including the carbon atoms of the bromophenyl group), being synperiplanar around the bond C9—N1 and antiperiplanar elsewhere. The interplanar angle to the plane of the benzothiazole unit (r.m.s. deviation 0.01 Å) is 69.75 (2)°. The coordination geometry at the nitrogen atom N1 of the NH group is planar (r.m.s. deviation of 4 atoms 0.003 Å).

3. Supramolecular features

The NH group at N1 is involved in a classical hydrogen bond to O1 via an inversion centre (Table 2), leading to the well-known motif with graph set $R_2^2(8)$. Three borderline 'weak' hydrogen bonds are also included in Table 2. There is a further

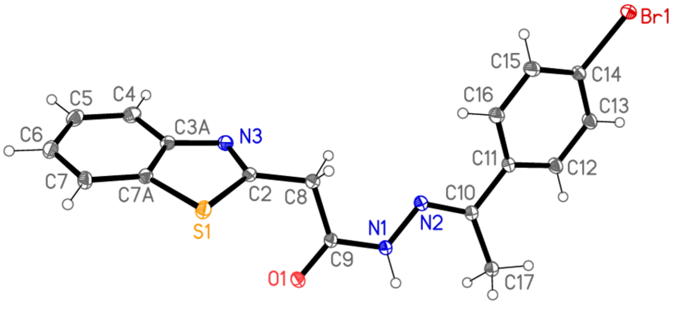


Figure 2
The molecule of compound **7** in the crystal. Ellipsoids correspond to 50% probability levels.

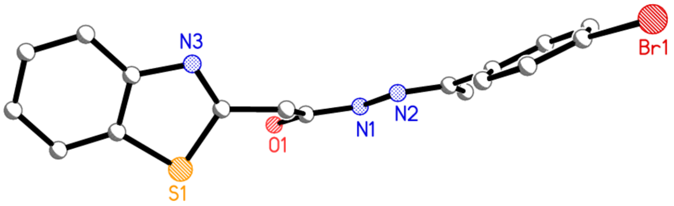


Figure 3
'Side view' of the molecule of **7**; hydrogen atoms are omitted and radii are arbitrary.

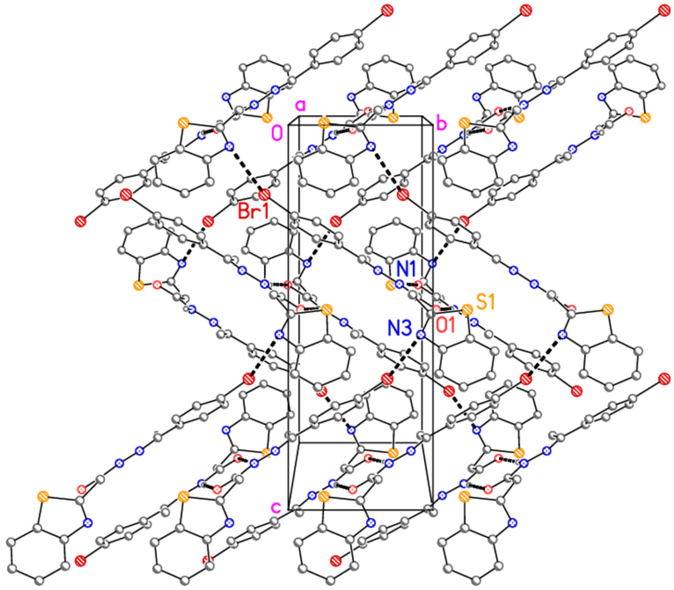


Figure 4
Packing diagram of compound **7**: One layer viewed perpendicular to the *bc* plane, showing classical hydrogen bonds (seen almost end-on, *cf.* Fig. 5) and halogen bonds (both as thick dashed lines). Hydrogen atoms not involved in the hydrogen bonding are omitted. Labels indicate atoms of the asymmetric unit.

contact N3···Br1 ($x, \frac{1}{2} - y, \frac{1}{2} + z$) of 3.1572 (10) Å, with an N···Br—C angle of 161.26 (4)°, that may be regarded as a 'halogen bond' [for reviews of this topic, see e.g. Cavallo *et al.* (2016) or Metrangolo *et al.* (2008)]. The combination of classical hydrogen bond plus halogen bond leads to the formation of a layer structure (Fig. 4) parallel to the *bc* plane and with a thickness equal to the length of the *a* axis. Because the hydrogen bonds are seen almost end-on in Fig. 4, a projection of the structure parallel to the *b* axis (Fig. 5) is also shown for the sake of clarity.

4. Database survey

Searches were conducted using CSD Version 6.00 (update August 2025; Groom *et al.*, 2016) and the ConQuest routine (Bruno *et al.*, 2002), Version 2025.2.0. The main search was based on the standard benzo[*d*]thiazole ring system with appropriately defined coordination numbers but no limitations on bond orders or on substituents except for that at C2; this substituent was set to $–C^4–C^3(–O^1)–N^{any}$ (as in **7**), where the superscripts indicate coordination number, whereby all bond orders in this fragment were allowed. This gave 18 hits. Only three of these structures had a 2-substituent of the type $–C^4–C^3(–O^1)–N^{any}–N^{any}$ (as in **7**): 4-(1,3-benzothiazol-2-yl)-5-methyl-2-phenyl-4-(prop-2-en-1-yl)-2,4-dihydro-3*H*-pyrazol-3-one (refcode DOMYAI: Chakib *et al.*, 2019) and our previous structures, the hydrazine derivatives *N*′-[(1,3-benzothiazol-2-yl)acetyl]benzohydrazide (IYUSIH; Azzam *et al.*, 2021) and 2-(1,3-benzothiazol-2-yl)-*N*′-[(4-methylphenyl)sulfonyl]acetohydrazide (JEBQOZ; Azzam *et al.*, 2017). Similarly, only three structures involved the 2-substituent $–CH_2–C^3(–O^1)–N^{any}$ (as in **7**), namely IYUSIH, JEBQOZ and 2-(1,3-benzothiazol-2-yl)-*N*-(2-hydroxyphenyl)acetamide (HANREW; Dauer *et al.*, 2017).

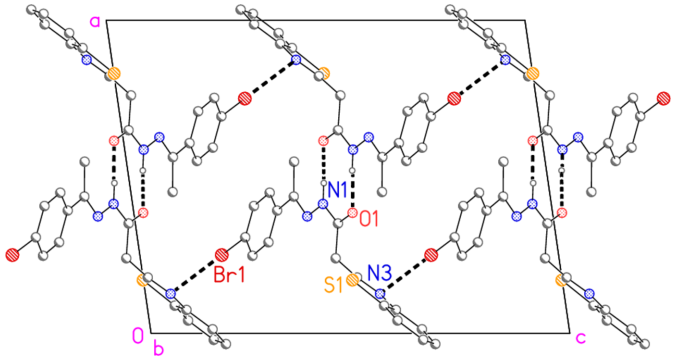


Figure 5
Simplified packing diagram of compound **7** shown as a projection parallel to the *b* axis.

Table 3
Experimental details.

Crystal data	
Chemical formula	$C_{17}H_{14}BrN_3OS$
M_r	388.28
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	100
a, b, c (Å)	13.4768 (3), 6.73234 (16), 17.8734 (5)
β (°)	98.169 (2)
V (Å^3)	1605.21 (7)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	2.70
Crystal size (mm)	0.25 × 0.10 × 0.04
Data collection	
Diffractometer	XtaLAB Synergy
Absorption correction	Multi-scan (*CrysAlis PRO*; Rigaku OD, 2024)
T_{min}, T_{max}	0.563, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	143532, 8606, 7894
R_{int}	0.063
θ values (°)	θ_{max} = 37.8, θ_{min} = 2.3
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.862
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.047, 0.085, 1.18
No. of reflections	8606
No. of parameters	213
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.44, −0.71

Computer programs: *CrysAlis PRO* (Rigaku OD, 2024), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2019/3* (Sheldrick, 2015*b*), *XP* (Bruker, 1998) and *publCIF* (Westrip, 2010).

5. Synthesis and crystallization

A mixture of 2-benzothiazolyl acetohydrazide **4** (2.072 g, 0.01 mol) and 4-bromophenylacetophenone **5** (3.98 g, 0.02 mol) was refluxed in ethanol (30 mL) for 3 h. The colourless solid product **7** thus formed was filtered from the

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hot solution, washed with a mixture of petroleum ether and ethyl acetate (1:1) and then recrystallized from ethanol.

Yellow solid; yield 80%; m.p. 466–468 K. IR (KBr, cm^{-1}): ν 3182 (NH), 3054 (Ar—CH), 1669 (CO); ^1H NMR (400 MHz, DMSO-d_6): δ 2.22 (*s*, 3H, CH_3), 4.36 (*s*, 2H, CH_2), 7.38–7.62 (*m*, 4H, Ar-H & benzothiazole-H), 7.74 (*d*, *J* = 8.4, 2H, Ar-H), 7.96 (*d*, *J* = 8.0 Hz, 1H, benzothiazole-H), 8.04 (*d*, *J* = 7.6 Hz, 1H, benzothiazole-H), 10.90 (*s*, 1H, NH). Analysis: calculated for $C_{17}H_{14}BrN_3OS$ (388.28): C 52.59, H 3.63, N 10.82. Found: C 52.53, H 3.60, N 10.81%.

6. Refinement

Details of data collection and structure refinement are summarized in Table 3. The benzothiazole system was assigned the standard IUPAC numbering. The hydrogen atom of the NH group was refined freely. The methyl group was refined as an idealized rigid group with C—H = 0.98 Å, H—C—H = 109.5°, allowed to rotate but not tip (AFIX 137). Other hydrogen atoms were included using a riding model starting from calculated positions ($C—H_{arom}$ = 0.95, $C—H_{methylene}$ = 0.98 Å). The U(H) values were fixed at 1.5 × U_{eq} of the parent carbon atoms for the methyl group and 1.2 × U_{eq} for the other hydrogens.

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Computing details

2-(Benzo[*d*]thiazol-2-yl)-*N′*-[(*E*)-1-(4-bromophenyl)ethylidene]acetohydrazide

Crystal data

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Monoclinic, $P2_1/c$
$a = 13.4768$ (3) Å
$b = 6.73234$ (16) Å
$c = 17.8734$ (5) Å
$\beta = 98.169$ (2)°
$V = 1605.21$ (7) Å^3
$Z = 4$

$F(000) = 784$
$D_x = 1.607$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 56121 reflections
$\theta = 2.3$–43.5°
$\mu = 2.70$ mm^{-1}
$T = 100$ K
Lath, colourless
0.25 × 0.10 × 0.04 mm

Data collection

XtaLAB Synergy diffractometer
Radiation source: micro-focus sealed X-ray tube, PhotonJet (Mo) X-ray Source
Mirror monochromator
Detector resolution: 10.0000 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlisPro; Rigaku OD, 2024)

$T_{min} = 0.563$, $T_{max} = 1.000$
143532 measured reflections
8606 independent reflections
7894 reflections with $I > 2\sigma(I)$
$R_{int} = 0.063$
$\theta_{max} = 37.8°$, $\theta_{min} = 2.3°$
$h = -23 \rightarrow 23$
$k = -11 \rightarrow 11$
$l = -30 \rightarrow 30$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.085$
$S = 1.18$
8606 reflections
213 parameters
0 restraints
Primary atom site location: dual

Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0311P)^2 + 1.1712P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 1.44$ e Å^{-3}
$\Delta\rho_{min} = -0.71$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
S1	0.16962 (2)	1.25918 (5)	0.49911 (2)	0.01614 (6)

C2	0.17813 (8)	1.00142 (18)	0.51133 (7)	0.01334 (18)
N3	0.12596 (8)	0.92656 (15)	0.56014 (6)	0.01357 (16)
C3A	0.07440 (8)	1.07504 (17)	0.59266 (7)	0.01226 (17)
C4	0.01259 (9)	1.0444 (2)	0.64826 (7)	0.0167 (2)
H4	0.003219	0.914827	0.667136	0.020*
C5	−0.03465 (10)	1.2067 (2)	0.67519 (8)	0.0185 (2)
H5	−0.076718	1.188063	0.712990	0.022*
C6	−0.02120 (9)	1.3985 (2)	0.64740 (8)	0.0176 (2)
H6	−0.055025	1.507238	0.666381	0.021*
C7	0.04045 (9)	1.43262 (19)	0.59281 (7)	0.0156 (2)
H7	0.049896	1.562658	0.574429	0.019*
C7A	0.08812 (8)	1.26853 (17)	0.56588 (7)	0.01244 (17)
C8	0.23962 (9)	0.8749 (2)	0.46650 (8)	0.0168 (2)
H8A	0.217578	0.898276	0.411983	0.020*
H8B	0.227229	0.733355	0.477020	0.020*
C9	0.35099 (8)	0.91582 (18)	0.48404 (7)	0.01371 (18)
O1	0.38489 (7)	1.05873 (16)	0.52236 (7)	0.0214 (2)
N1	0.41315 (8)	0.78849 (16)	0.45479 (7)	0.01472 (17)
H01	0.4799 (18)	0.818 (3)	0.4639 (13)	0.028 (6)*
N2	0.37355 (8)	0.62797 (16)	0.41312 (6)	0.01411 (17)
C10	0.43690 (9)	0.51041 (18)	0.38756 (7)	0.01316 (18)
C11	0.39222 (9)	0.33802 (17)	0.34310 (7)	0.01298 (18)
C12	0.44925 (9)	0.17000 (18)	0.33140 (7)	0.01525 (19)
H13	0.517977	0.165244	0.352572	0.018*
C13	0.40666 (9)	0.00945 (19)	0.28910 (7)	0.0158 (2)
H14	0.445809	−0.104428	0.281831	0.019*
C14	0.30657 (9)	0.01796 (18)	0.25778 (7)	0.01412 (18)
Br1	0.24979 (2)	−0.19335 (2)	0.19566 (2)	0.01864 (4)
C15	0.24758 (9)	0.1824 (2)	0.26853 (8)	0.0181 (2)
H16	0.179047	0.186459	0.246826	0.022*
C16	0.29056 (9)	0.34051 (19)	0.31154 (8)	0.0171 (2)
H17	0.250470	0.452312	0.319744	0.021*
C17	0.54844 (9)	0.5433 (2)	0.40014 (8)	0.0166 (2)
H11A	0.564414	0.664090	0.373666	0.025*
H11B	0.582002	0.429331	0.380591	0.025*
H11C	0.571579	0.557948	0.454370	0.025*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.01733 (12)	0.01212 (11)	0.02066 (14)	0.00074 (9)	0.00852 (10)	0.00166 (10)
C2	0.0104 (4)	0.0123 (4)	0.0171 (5)	0.0004 (3)	0.0012 (3)	−0.0023 (4)
N3	0.0124 (4)	0.0112 (4)	0.0167 (4)	0.0010 (3)	0.0007 (3)	0.0009 (3)
C3A	0.0112 (4)	0.0119 (4)	0.0133 (4)	0.0005 (3)	0.0005 (3)	0.0013 (3)
C4	0.0156 (4)	0.0188 (5)	0.0161 (5)	−0.0014 (4)	0.0032 (4)	0.0030 (4)
C5	0.0149 (4)	0.0250 (6)	0.0162 (5)	−0.0006 (4)	0.0048 (4)	−0.0010 (5)
C6	0.0142 (4)	0.0208 (5)	0.0178 (5)	0.0029 (4)	0.0025 (4)	−0.0036 (4)
C7	0.0155 (4)	0.0131 (4)	0.0181 (5)	0.0030 (4)	0.0022 (4)	−0.0011 (4)

C7A	0.0116 (4)	0.0113 (4)	0.0145 (5)	0.0010 (3)	0.0022 (3)	0.0005 (3)
C8	0.0114 (4)	0.0165 (5)	0.0226 (6)	−0.0001 (4)	0.0021 (4)	−0.0074 (4)
C9	0.0111 (4)	0.0137 (4)	0.0163 (5)	0.0006 (3)	0.0018 (3)	−0.0037 (4)
O1	0.0125 (3)	0.0209 (4)	0.0306 (5)	−0.0009 (3)	0.0026 (3)	−0.0145 (4)
N1	0.0116 (4)	0.0138 (4)	0.0191 (5)	−0.0003 (3)	0.0031 (3)	−0.0059 (3)
N2	0.0135 (4)	0.0134 (4)	0.0156 (4)	−0.0002 (3)	0.0024 (3)	−0.0038 (3)
C10	0.0131 (4)	0.0133 (4)	0.0132 (4)	0.0003 (3)	0.0026 (3)	−0.0025 (4)
C11	0.0136 (4)	0.0126 (4)	0.0129 (4)	0.0001 (3)	0.0026 (3)	−0.0021 (3)
C12	0.0145 (4)	0.0143 (5)	0.0164 (5)	0.0021 (3)	0.0000 (4)	−0.0032 (4)
C13	0.0165 (4)	0.0133 (4)	0.0171 (5)	0.0019 (4)	0.0012 (4)	−0.0031 (4)
C14	0.0159 (4)	0.0130 (4)	0.0140 (5)	−0.0026 (3)	0.0036 (4)	−0.0029 (4)
Br1	0.01679 (5)	0.01735 (6)	0.02281 (7)	−0.00640 (4)	0.00638 (4)	−0.00819 (5)
C15	0.0133 (4)	0.0176 (5)	0.0228 (6)	−0.0006 (4)	0.0006 (4)	−0.0050 (4)
C16	0.0134 (4)	0.0151 (5)	0.0225 (6)	0.0013 (4)	0.0015 (4)	−0.0053 (4)
C17	0.0126 (4)	0.0186 (5)	0.0187 (5)	−0.0004 (4)	0.0027 (4)	−0.0068 (4)

Geometric parameters (Å, º)

S1—C7A	1.7342 (12)	C12—C13	1.3950 (17)
S1—C2	1.7507 (12)	C13—C14	1.3862 (17)
C2—N3	1.2976 (16)	C14—C15	1.3919 (18)
C2—C8	1.4977 (17)	C14—Br1	1.8975 (12)
N3—C3A	1.3909 (16)	C15—C16	1.3905 (18)
C3A—C4	1.3998 (17)	C4—H4	0.9500
C3A—C7A	1.4090 (17)	C5—H5	0.9500
C4—C5	1.385 (2)	C6—H6	0.9500
C5—C6	1.405 (2)	C7—H7	0.9500
C6—C7	1.3875 (19)	C8—H8A	0.9900
C7—C7A	1.3973 (17)	C8—H8B	0.9900
C8—C9	1.5144 (16)	N1—H01	0.91 (2)
C9—O1	1.2307 (15)	C12—H13	0.9500
C9—N1	1.3543 (15)	C13—H14	0.9500
N1—N2	1.3764 (15)	C15—H16	0.9500
N2—C10	1.2942 (15)	C16—H17	0.9500
C10—C11	1.4849 (17)	C17—H11A	0.9800
C10—C17	1.5044 (17)	C17—H11B	0.9800
C11—C12	1.3999 (17)	C17—H11C	0.9800
C11—C16	1.4057 (17)		

C7A—S1—C2	89.24 (6)	C16—C15—C14	118.95 (11)
N3—C2—C8	122.18 (11)	C15—C16—C11	121.23 (11)
N3—C2—S1	115.90 (9)	C5—C4—H4	120.7
C8—C2—S1	121.90 (9)	C3A—C4—H4	120.7
C2—N3—C3A	110.63 (10)	C4—C5—H5	119.5
N3—C3A—C4	125.01 (11)	C6—C5—H5	119.5
N3—C3A—C7A	115.16 (10)	C7—C6—H6	119.3
C4—C3A—C7A	119.84 (11)	C5—C6—H6	119.3
C5—C4—C3A	118.66 (12)	C6—C7—H7	121.2

C4—C5—C6	120.91 (12)	C7A—C7—H7	121.2
C7—C6—C5	121.40 (12)	C2—C8—H8A	108.9
C6—C7—C7A	117.51 (12)	C9—C8—H8A	108.9
C7—C7A—C3A	121.67 (11)	C2—C8—H8B	108.9
C7—C7A—S1	129.27 (10)	C9—C8—H8B	108.9
C3A—C7A—S1	109.07 (8)	H8A—C8—H8B	107.8
C2—C8—C9	113.15 (10)	C9—N1—H01	116.1 (15)
O1—C9—N1	120.57 (11)	N2—N1—H01	124.4 (15)
O1—C9—C8	122.41 (11)	C13—C12—H13	119.5
N1—C9—C8	117.01 (10)	C11—C12—H13	119.5
C9—N1—N2	119.49 (10)	C14—C13—H14	120.4
C10—N2—N1	116.53 (10)	C12—C13—H14	120.4
N2—C10—C11	115.41 (10)	C16—C15—H16	120.5
N2—C10—C17	123.54 (11)	C14—C15—H16	120.5
C11—C10—C17	121.04 (10)	C15—C16—H17	119.4
C12—C11—C16	118.30 (11)	C11—C16—H17	119.4
C12—C11—C10	121.47 (10)	C10—C17—H11A	109.5
C16—C11—C10	120.23 (10)	C10—C17—H11B	109.5
C13—C12—C11	120.98 (11)	H11A—C17—H11B	109.5
C14—C13—C12	119.25 (11)	C10—C17—H11C	109.5
C13—C14—C15	121.28 (11)	H11A—C17—H11C	109.5
C13—C14—Br1	119.58 (9)	H11B—C17—H11C	109.5
C15—C14—Br1	119.09 (9)		

C7A—S1—C2—N3	−0.02 (10)	C2—C8—C9—O1	−10.43 (19)
C7A—S1—C2—C8	178.31 (10)	C2—C8—C9—N1	170.32 (12)
C8—C2—N3—C3A	−178.76 (11)	O1—C9—N1—N2	178.97 (12)
S1—C2—N3—C3A	−0.44 (13)	C8—C9—N1—N2	−1.76 (18)
C2—N3—C3A—C4	−178.97 (12)	C9—N1—N2—C10	−179.12 (12)
C2—N3—C3A—C7A	0.82 (14)	N1—N2—C10—C11	179.74 (11)
N3—C3A—C4—C5	−179.62 (12)	N1—N2—C10—C17	−1.04 (19)
C7A—C3A—C4—C5	0.60 (18)	N2—C10—C11—C12	−160.60 (12)
C3A—C4—C5—C6	0.1 (2)	C17—C10—C11—C12	20.16 (18)
C4—C5—C6—C7	−0.7 (2)	N2—C10—C11—C16	19.43 (18)
C5—C6—C7—C7A	0.57 (19)	C17—C10—C11—C16	−159.82 (12)
C6—C7—C7A—C3A	0.15 (18)	C16—C11—C12—C13	0.41 (19)
C6—C7—C7A—S1	−179.52 (10)	C10—C11—C12—C13	−179.56 (12)
N3—C3A—C7A—C7	179.45 (11)	C11—C12—C13—C14	0.6 (2)
C4—C3A—C7A—C7	−0.75 (18)	C12—C13—C14—C15	−0.8 (2)
N3—C3A—C7A—S1	−0.82 (13)	C12—C13—C14—Br1	176.63 (10)
C4—C3A—C7A—S1	178.98 (9)	C13—C14—C15—C16	0.1 (2)
C2—S1—C7A—C7	−179.84 (12)	Br1—C14—C15—C16	−177.39 (11)
C2—S1—C7A—C3A	0.46 (9)	C14—C15—C16—C11	1.0 (2)
N3—C2—C8—C9	−115.73 (13)	C12—C11—C16—C15	−1.2 (2)
S1—C2—C8—C9	66.05 (14)	C10—C11—C16—C15	178.79 (13)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H01···O1^{i}	0.91 (2)	1.98 (2)	2.8839 (14)	168 (2)
C7—H7···N3^{ii}	0.95	2.68	3.5942 (17)	161
C17—H11*B*···Br1^{iii}	0.98	2.93	3.7666 (12)	145
C17—H11*C*···N2^{iv}	0.98	2.69	3.5464 (18)	147

Symmetry codes: (i) $-x+1, -y+2, -z+1$; (ii) $x, y+1, z$; (iii) $-x+1, y+1/2, -z+1/2$; (iv) $-x+1, -y+1, -z+1$.